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A new approach to solution of the light scattering problems for particles with a symmetry plane by using the field expansions in wave functions

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Solving the light scattering problem for particles with the middle symmetry plane (e.g., spheroids), by applying the exact methods based on the field expansions in basis functions, leads to the linear systems with half matrix elements equal to zero. We suggest an approach that allows one to replace such a system with two ones having a twice smaller size, which significantly reduces the computational time. The approach is applied to the recently derived solution to the light scattering problem for homogeneous spheroids with the field expansions in spheroidal functions. The approach can be used in the case of the field expansions in spherical and other functions as well as for other scatterers, e.g., finite length cylinders, Chebyshev particles with the even parameter n, and so on, including both homogeneous and layered ones.

Keywords: light scattering, spheroidal scatterers, T-matrix.

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1. Introduction

The approximation of real scatterers by particles of simple shapes is quite often encountered in various applications of the theory of light scattering [1–3]. The implementation of such an approach in many cases requires a quick solution to the problem of scattering of a plane electromagnetic wave incident on a particle of the corresponding (non-spherical) shape.

Numerical solutions to this problem obtained by universal methods (for example, discrete dipole approximation, DDA, finite difference time domain method, FDTD, etc. [4,5]) often require very long computation time and thus, are significantly limited in application.

Solutions based on the field expansion on a selected basis as part of different methods (separation of variables method, SVM, extended boundary condition method, EBCM, etc. [6]) have a wider range of applicability. Here, when reviewing particles with a large diffraction parameter, etc., as a rule, it is required to take into account many terms of the expansion, i. e. large linear systems need to be solved. Since in this case the computation time grows approximately as N^4, where N — the order of the system matrix, reducing this parameter can give a significant acceleration

This effect, in particular, can be expected when dividing a system of equations for relatively unknown field expansion coefficients into two systems, half the size, which is possible for particles with a median plane of symmetry. As is known, in this case the matrix of the system contains half of the zero elements [7], and their elimination is equivalent to splitting the system into two parts with matrices not containing such elements.

In this work we review the application of a similar approach to solving the problem of light scattering by a homogeneous spheroid, which we recently obtained using the EBCM method applying field expansions in spheroidal functions and described in detail in the work [8]. The basic elements of solving the problem in [8] are briefly presented in Section 2. The proposed new approach is described in Section 3, some data from numerical calculations are presented and the actual acceleration of calculations are discussed in Section 4. The results of this work are summarized in the Conclusion.

2. General relations

In the work [8], as usual in the EBCM method, not the Helmholtz (wave) equations for harmonic fields $\mathbf{E}$, $\mathbf{H}$ were solved together with boundary conditions [1], but the surface integral equations equivalent to them, often called extended boundary condition,

$$\nabla\times\int\limits_S \mathbf{n}\times\mathbf{E}^{\mathrm{int}}(\mathbf{r}')G(\mathbf{r},\mathbf{r}')ds' - \frac{1}{ik\varepsilon}\nabla\times\nabla$$
$$\times\int_S \mathbf{n}\times\mathbf{H}^{\mathrm{int}}(\mathbf{r}')G(\mathbf{r},\mathbf{r}')ds'$$
$$=\begin{cases}-\mathbf{E}^{\mathrm{int}}(\mathbf{r}), & \mathbf{r}\in D,\\ \mathbf{E}^{\mathrm{sca}}(\mathbf{r}), & \mathbf{r}\in\bar{D}\setminus S,\end{cases} \tag{1}$$

where $G(\mathbf{r},\mathbf{r}')=\exp(ik_0|\mathbf{r}-\mathbf{r}'|)/(4\pi|\mathbf{r}-\mathbf{r}'|)$ is Green's function of the scalar Helmholtz equation for free space, $k_0=2\pi/\lambda$ — wave number in vacuum, λ — radiation wavelength, S — particle surface, $\mathbf{n}$ — outer normal to S, D — region inside S, ε and μ — dielectric permittivity and magnetic susceptibility of the medium, while $k=k_0\sqrt{\varepsilon\mu}$ — wave number in the medium, $\mathbf{E}^{\text{in}}$ and $\mathbf{E}^{\text{sca}}$ — fields of incident and scattered radiation, respectively, $\mathbf{E}^{\text{int}}, \mathbf{H}^{\text{int}}$ — field inside particles.

Electromagnetic fields were represented in infinite series as follows:

$$\mathbf{E}(\mathbf{r})=\sum_{\nu}\left(a_\nu\mathbf{M}^{\text{s}}_\nu(\mathbf{r})+b_\nu\mathbf{N}^{\text{s}}_\nu(\mathbf{r})\right), \tag{2}$$

where a_ν and b_ν — expansion coefficients, and $\mathbf{M}^{\text{s}}_\nu(\mathbf{r})$, $\mathbf{N}^{\text{s}}_\nu(\mathbf{r})$ — basis functions, which are solutions of the Helmholtz equation that satisfy the required conditions,

$$\mathbf{M}^{\text{s}}_\nu(\mathbf{r})=\nabla\times(\mathbf{s}\psi_\nu(\mathbf{r})),\qquad \mathbf{N}^{\text{s}}_\nu(\mathbf{r})=\frac{1}{k}\nabla\times\mathbf{M}^{\text{s}}_\nu(\mathbf{r}), \tag{3}$$

where $\mathbf{s}$ is either the radius vector $\mathbf{r}$ or the unit vector $\mathbf{i}_z$, and ψ_ν is a solution to the corresponding scalar Helmholtz equation.

In the spheroidal coordinate system (ξ,η,φ) we have

$$\overline{\psi}^{(j)}_\nu(\xi,\eta,\varphi)=\tilde{c}_{mn}R^{(j)}_{mn}(c,\xi)\overline{S}_{mn}(c,\eta)\mathrm{e}^{im\varphi}, \tag{4}$$

where $\nu=\{m,n\}$, $n=0,\ 1,\ldots,$ $m=-n,\ldots,n$, $\tilde{c}_{mn}$ — some coefficient of order 1, $R^{(j)}_{mn}(c,\xi)$ — spheroidal radial functions of the j-th kind $(j=1,3)$. The parameter c is equal to $kd/2$ and $-ikd/2$ for prolate and oblate spheroidal coordinates, respectively, d — their focal distance [9]. Normalized spheroidal angular functions $\overline{S}_{mn}(c,\eta)=S_{mn}(c,\eta)/N_{mn}$ were used, where $N_{mn}=[2(n+m)!/(2n+1)/(n-m)!]^{1/2}$ according to [10]. The solution is somewhat simplified if trigonometric functions φ are used in formula (4), as is done below. Then the concepts of TE- and TM-mode, etc. [8] appear. Note that in expansion (2) we use the functions in the TM mode $\mathbf{M}^{\mathbf{r}}_\nu$, $\mathbf{M}^{\mathbf{z}}_\nu$, and in TE mode — $\mathbf{N}^{\mathbf{r}}_\nu$, $\mathbf{N}^{\mathbf{z}}_\nu$.

The spheroidal coordinate system is naturally associated with the surface of the spheroidal particle, so that the coordinate ξ at its boundary is constant. Then substitution of relations (2)−(4) and the known expansion of the Green's function [11] into equation (1) taking into account the properties of spheroidal functions leads in a standard way to a system of linear algebraic equations

$$\begin{cases}\mathbf{Z}^{\text{in}}=-\tilde{A}_{31}\mathbf{Z}^{\text{int}},\\ \mathbf{Z}^{\text{sca}}=\tilde{A}_{11}\mathbf{Z}^{\text{int}}.\end{cases} \tag{5}$$

Here the vectors have two parts (in accordance with expansion (2)): $\mathbf{Z}^{\text{in}}=\left\{\mathbf{Z}^{\text{in}}_{\text{U}},\mathbf{Z}^{\text{in}}_{\text{V}}\right\}^T$, $\mathbf{Z}^{\text{int}}=\left\{\mathbf{Z}^{\text{int}}_{\text{U}},\mathbf{Z}^{\text{int}}_{\text{V}}\right\}^T$, $\mathbf{Z}^{\text{sca}}=\left\{\mathbf{Z}^{\text{sca}}_{\text{U}},\mathbf{Z}^{\text{sca}}_{\text{V}}\right\}^T$ with the components

$$z^{\text{in}}_{\text{U},ml}=k_1\overline{a}^{\text{in}}_{ml}R^{(1)}_{ml}(c_1,\xi_0),\quad z^{\text{in}}_{\text{U},ml}=0,$$

$$z^{\text{int}}_{\text{U},ml}=k_1\overline{a}^{\text{int}}_{ml}R^{(1)}_{ml}(c_2,\xi_0),$$
$$z^{\text{int}}_{\text{V},ml}=c_1\overline{b}^{\text{int}}_{ml}R^{(1)}_{ml}(c_2,\xi_0),$$
$$z^{\text{sca}}_{\text{U},ml}=k_1\overline{a}^{\text{sca}}_{ml}R^{(3)}_{ml}(c_1,\xi_0),$$
$$z^{\text{sca}}_{\text{V},ml}=c_1\overline{b}^{\text{sca}}_{ml}R^{(3)}_{ml}(c_1,\xi_0), \tag{6}$$

where ξ_0 — the value of the coordinate ξ on the surface S, c_1 and c_2 — the value of the parameter c outside and inside the particle, k_1 — the wave number in the medium surrounding the particle.

Let us note that for axisymmetric particles the operator corresponding to the light scattering problem commutes with the rotation operator $L_z=\partial/\partial\varphi$, which allows to divide the problem with respect to one of the variables — the azimuthal angle φ, i.e. the problem can be solved independently for each value of the azimuthal number m [6]. Although all vectors and matrices below should have index m (as in [8]), we omit it for simplicity in all but a few cases.

Both matrices in the system (5) have 4 blocks ($i=1,3$; $k=1$)

$$\tilde{A}_{ik}=\begin{pmatrix}\alpha_{\text{U},ik} & \alpha_{\text{V},ik}\\ \beta_{\text{U},ik} & \beta_{\text{V},ik}\end{pmatrix}. \tag{7}$$

In the work [8] the expressions of the matrix elements in formula (7) for the TE mode are given. We review the case of the TM mode below, for simplicity, but without loss of generality. The transition from the first to the second mode occurs by cyclic replacement: $\varepsilon\to\mu$, $\mu\to\varepsilon$. With the usual values of the magnetic susceptibility of $\mu_1=\mu_2=1$ media for $\tilde{A}_{31}$ elements in the TM mode, we obtain

$$\alpha_{\text{U},31}=W\left\{R_{3,1}\Delta_{1,2}-\frac{\varepsilon_1}{\varepsilon_2}\Delta_{1,2}R_{1,2}+\left(\frac{\varepsilon_1}{\varepsilon_2}-1\right)\right.$$
$$\left.\times\ \xi_0^2Q_{1,2}R_{1,2}-\left(1-\frac{\varepsilon_1}{\varepsilon_2}\right)\frac{f\xi_0}{\xi_0^2-f}Q_{1,2}E_{2,2}\right\}, \tag{8}$$

$$\alpha_{\text{V},31}=W\left\{\left(\frac{\varepsilon_1}{\varepsilon_2}-1\right)f\xi_0Q_{1,2}\Gamma_{2,2}R_{1,2}-\left(1-\frac{\varepsilon_1}{\varepsilon_2}\right)\right.$$
$$\left.\times\frac{f}{\xi_0^2-f}\left[\left(\xi_0^2Q_{1,2}-\Delta_{1,2}\right)K_{2,2}+\Gamma_{1,2}\right]\right\}, \tag{9}$$

$$\beta_{\text{U},31}=W\left\{-\left(\frac{\varepsilon_1}{\varepsilon_2}-1\right)\xi_0Q_{1,2}\Gamma_{2,2}R_{1,2}\right.$$
$$\left.+\left(1-\frac{\varepsilon_1}{\varepsilon_2}\right)\frac{\xi_0^2}{\xi_0^2-f}Q_{1,2},K_{2,2}\right\}, \tag{10}$$

$$\beta_{\text{V},31}=W\left\{R_{3,1}\Delta_{1,2}-\Delta_{1,2}R_{1,2}-\left(\frac{\varepsilon_1}{\varepsilon_2}-1\right)\right.$$
$$\left.\times\xi_0^2Q_{1,2}R_{1,2}+\left(1-\frac{\varepsilon_1}{\varepsilon_2}\right)\frac{\xi_0}{\xi_0^2-f}\left[Q_{1,2}E_{2,2}+\Delta_{1,2}\right]\right\}, \tag{11}$$

where ε_1 and ε_2 — dielectric permittivity outside and inside the particle, $f=-1$ and 1 for oblate and prolate spheroidal coordinates, I — unit matrix. The elements of the matrix $\tilde{A}_{11}$ look similar [8].

With our choice of spheroidal coordinates, the radial functions used are constant on the surface of the particle and, therefore, are taken out of the sign of the integral over its surface in the matrix elements in system (5). Therefore, such functions are present only in the following diagonal matrices:

$$R_{k,j} = \left\{ \frac{R_{ml}^{(k)'}(c_j, \xi_0)}{R_{ml}^{(k)}(c_j, \xi_0)} \delta_{nl} \right\}_{n,l=m}^{\infty}, \qquad (12)$$

$$W = -\left[R_{3,1} - R_{1,1}\right]^{-1} = \left\{ i c_1(\xi_0^2 - f) R_{ml}^{(1)}(c_1, \xi_0) R_{ml}^{(3)}(c_1, \xi_0) \delta_{nl} \right\}_{n,l=m}^{\infty}, \qquad (13)$$

where $R_{ml}^{(k)'}(c, \xi)$ — derivative of the spheroidal radial function of the k-th kind, δ_{nl} — Kronecker symbol, $k = 1, 3$ and $j = 1, 2$.

The elements of the matrices $\Delta_{i,j}$, $\Gamma_{i,j}$, $K_{i,j}$, $E_{i,j}$ $(i = 1, 2;\ j = 1, 2)$ represent, respectively, the following integrals of normalized spheroidal angular functions and their derivatives:

$$\delta_{nl}(c_i, c_j) = \int_{-1}^{1} \bar{S}_{mn}(c_i, \eta) \bar{S}_{ml}(c_j, \eta)\, d\eta, \qquad (14)$$

$$\gamma_{nl}(c_i, c_j) = \int_{-1}^{1} \bar{S}_{mn}(c_i, \eta)\, \bar{S}_{ml}(c_j, \eta)\, \eta\, d\eta, \qquad (15)$$

$$\kappa_{nl}(c_i, c_j) = \int_{-1}^{1} \bar{S}'_{mn}(c_i, \eta)\, \bar{S}_{ml}(c_j, \eta)(1 - \eta^2)\, d\eta, \qquad (16)$$

$$\varepsilon_{nl}(c_i, c_j) = \int_{-1}^{1} \bar{S}'_{mn}(c_i, \eta)\, \bar{S}_{ml}(c_j, \eta)\, (1 - \eta^2)\, \eta\, d\eta, \qquad (17)$$

where $n,\ l = m,\ m+1, \ldots$

Finally,

$$Q_{1,2} = \Delta_{1,2} \left[\xi_0^2 I - f \Gamma^2(c_2, c_2)\right]^{-1}. \qquad (18)$$

In the case of a single particle, solving system (5), we obtain the elements $z_{\mathrm{U},ml}^{\mathrm{sca}}$, $z_{\mathrm{V},ml}^{\mathrm{sca}}$ and then the expansion coefficients (2) of the scattered field $\bar{a}_{ml}^{\mathrm{sca}}$, $\bar{b}_{ml}^{\mathrm{sca}}$. These data allow to find any cross sections and scattering matrix for a given particle [8].

On the other hand, for ensembles of particles (in particular, chaotically oriented ones) from the matrices of system (5), one can construct an analogue of the T matrix: $\tilde{T} = \tilde{A}_{11}(\tilde{A}_{31})^{-1}$which in general has $4\tilde{T}_{ij}$ $(i,\ j = 1, 2)$ blocks:

$$\begin{pmatrix} \mathbf{Z}_{\mathrm{U}}^{\mathrm{sca}} \\ \mathbf{Z}_{\mathrm{V}}^{\mathrm{sca}} \end{pmatrix} = \begin{pmatrix} \tilde{T}_{11} & \tilde{T}_{12} \\ \tilde{T}_{21} & \tilde{T}_{22} \end{pmatrix} \begin{pmatrix} \mathbf{Z}_{\mathrm{U}}^{\mathrm{in}} \\ 0 \end{pmatrix}. \qquad (19)$$

This allows to define 2 blocks of a normalized spheroidal T matrix (TM mode case)

$$\bar{\mathbf{a}}^{\mathrm{sca}} = -\bar{T}_{11}^{\mathrm{sp}} \bar{\mathbf{a}}^{\mathrm{in}}, \qquad \bar{\mathbf{b}}^{\mathrm{sca}} = -\bar{T}_{21}^{\mathrm{sp}} \bar{\mathbf{a}}^{\mathrm{in}}, \qquad (20)$$

where

$$\bar{T}_{11}^{\mathrm{sp}} = \tilde{R}_3^{-1} \tilde{T}_{11} \tilde{R}_1, \quad \bar{T}_{21}^{\mathrm{sp}} = \frac{k_1}{c_1} \tilde{R}_3^{-1} \tilde{T}_{21} \tilde{R}_1, \qquad (21)$$

diagonal matrices $\tilde{R}_i = \left\{ R_{mn}^{(i)}(c_1, \xi_0) \delta_{nl} \right\}_{n,l=m}^{\infty}$.

Based on $\bar{T}^{\mathrm{sp}}$, in the work [8] a standard T matrix was constructed that relates the scattered and incident fields expansion coefficients on a certain spherical basis and fundamentally accelerates the calculation of the optical properties of ensembles of (chaotically oriented) particles [4].

3. Description of the proposed approach

The new approach uses the fact that for particles with a plane of symmetry, with a suitable choice of basis in the SVM, EBCM, etc. methods, half of the matrix elements in emerging systems of linear algebraic equations with respect to unknown field expansion coefficients, which are essentially similar to the system (5), turn out to be zero.

This feature of systems is associated with the oddness of angular functions. For example, in the case described in Section 2, the matrix elements include the integrals (14)−(17). The functions $\bar{S}_{mn}(c, \eta)$ and $\eta\, \bar{S}'_{mn}(c, \eta)$ included in these integrals are even and odd functions η when the difference $n - m$ is even and odd, correspondingly [9]. Therefore, regardless of m, the integrals $\delta_{nl}(c_1, c_2)$ and $\varepsilon_{nl}(c_1, c_2)$ are zero when $n - l$ is odd, and the integrals $\gamma_{nl}(c_1, c_2)$ and $\kappa_{nl}(c_1, c_2)$ are zero when $n - l$ is even.

As a consequence, the $\tilde{A}_{31}$, $\tilde{A}_{11}$ matrices in system (5) contain two types of matrices involving spheroidal angular functions: matrices like Δ and Γ. In the first case (matrices Δ, E, Q), elements the indices of which have different parities are equal to zero, and in the second (Γ, K) — the same (8)−(11) and (14)−(17).

For Δ-type matrices, the reduced matrices can be entered that do not contain zeros as follows:

$$\Delta_1 = \begin{pmatrix} \delta_{11} & \delta_{13} & \ldots \\ \delta_{31} & \delta_{33} & \ldots \\ \ldots & \ldots & \ldots \end{pmatrix}, \quad \Delta_2 = \begin{pmatrix} \delta_{22} & \delta_{24} & \ldots \\ \delta_{42} & \delta_{44} & \ldots \\ \ldots & \ldots & \ldots \end{pmatrix}. \qquad (22)$$

These matrices are obtained by deleting even rows and columns in the first case, and odd ones in the second. Let us note that the matrices are almost symmetric: $\delta_{nl}(c_1, c_2) = \delta_{ln}(c_2, c_1)$.

For Γ-type matrices, the reduced analogues respectively have the form

$$\Gamma_1 = \begin{pmatrix} \gamma_{12} & \gamma_{14} & \ldots \\ \gamma_{32} & \gamma_{34} & \ldots \\ \ldots & \ldots & \ldots \end{pmatrix},$$

$$\Gamma_2 = \begin{pmatrix} \gamma_{21} & \gamma_{23} & \cdots \\ \gamma_{41} & \gamma_{43} & \cdots \\ \cdots & \cdots & \cdots \end{pmatrix}. \tag{23}$$

In this case, to obtain matrices Γ_1, even rows and odd columns are crossed out in matrix Γ, and odd rows and even columns are excluded to obtain Γ_2. These integrals are also related $\gamma_{nl}(c_1, c_2) = \gamma_{ln}(c_2, c_1)$.

Thus, in system (5) it is advisable to divide the vectors of coefficients $\mathbf{Z}_X^Y$ for each upper and lower indices (X =U,V; Y = in, int, sca) into two: $\mathbf{Z}_{1,X}^Y$ and $\mathbf{Z}_{2,X}^Y$, thinning out parts of $\mathbf{Z}_X^Y$ in different ways. The components of the new vectors for each m are equal to

$$z_{1,X,ml}^{Y} = z_{X,ml}^{Y}, \qquad l = m,\ m+2, \ldots, \tag{24}$$

$$z_{2,X,ml}^{Y} = z_{X,\,ml}^{Y}, \qquad l = m+1, m+3, \ldots, \tag{25}$$

where the right-hand sides are similar to those given in relations (6).

Then, for example, the first equation of system (5) splits into two ($j = 1, 2$) equations:

$$\begin{pmatrix} -\alpha_{j,U,31} & -\alpha_{3-j,V,31} \\ -\beta_{3-j,U,31} & -\beta_{j,V,31} \end{pmatrix} \begin{pmatrix} \mathbf{Z}_{j,U}^{int} \\ \mathbf{Z}_{3-j,V}^{int} \end{pmatrix} = \begin{pmatrix} \mathbf{Z}_{j,U}^{in} \\ 0 \end{pmatrix}. \tag{26}$$

For the TM mode, under the condition $\mu_1 = \mu_2 = 1$, we respectively have ($j = 1, 2$)

$$\alpha_{j,U,31} = W_j \left\{ R_{j,3,1}\Delta_{j,1,2} - \frac{\varepsilon_1}{\varepsilon_2}\Delta_{j,1,2}R_{j,1,2} + \left(\frac{\varepsilon_1}{\varepsilon_2} - 1\right) \times \xi_0^2 Q_{j,1,2}R_{j,1,2} - \left(1 - \frac{\varepsilon_1}{\varepsilon_2}\right) \frac{f\xi_0}{\xi_0^2 - f} Q_{j,1,2}E_{j,2,2} \right\}, \tag{27}$$

$$\alpha_{j,V,31} = W_{3-j} \left\{ f\xi_0 Q_{j,1,2}\Gamma_{j,2,2}R_{3-j,1,2} - \left(1 - \frac{\varepsilon_1}{\varepsilon_2}\right) \times \frac{f}{\xi_0^2 - f} \left[\left(\xi_0^2 Q_{j,1,2} - \Delta_{j,1,2}\right) K_{j,2,2} + \Gamma_{j,1,2} \right] \right\}, \tag{28}$$

$$\beta_{j,U,31} = W_j \left\{ -\left(\frac{\varepsilon_1}{\varepsilon_2} - 1\right) \xi_0 Q_{3-j,1,2}\Gamma_{3-j,2,2}R_{j,1,2} + \left(1 - \frac{\varepsilon_1}{\varepsilon_2}\right) \frac{\xi_0^2}{\xi_0^2 - f} Q_{3-j,1,2}K_{3-j,2,2} \right\}, \tag{29}$$

$$\beta_{j,V,31} = W_{3-j} \left\{ R_{3-j,3,1}\Delta_{3-j,1,2} - \Delta_{3-j,1,2}R_{3-j,1,2} - \left(\frac{\varepsilon_1}{\varepsilon_2} - 1\right) \xi_0^2 Q_{3-j,1,2}R_{3-j,1,2} \left(1 - \frac{\varepsilon_1}{\varepsilon_2}\right) \times \frac{\xi_0}{\xi_0^2 - f} \left[Q_{3-j,1,2}E_{3-j,2,2} + \Delta_{3-j,1,2} \right] \right\}. \tag{30}$$

Obviously, the R_{ik} diagonal matrices must contain either the 1st, 3rd, etc. rows (this will be a matrix $R_{1,ik} = \{(r_{ik})_{nl}\}_{n,l=m,m+2,\ldots}$), the 2nd, 4th, etc. rows (matrix $R_{2,ik} = \{(r_{ik})_{nl}\}_{n,l=m+1,m+3,\ldots}$). The matrices W_1 and W_2 are constructed in a similar way.

Also, the second equation of the system (5) splits into two equations when using the variables $\mathbf{Z}_{1,X}^Y$ and $\mathbf{Z}_{2,X}^Y$ ($X = U, V$; $Y = \text{in, int, sca}$).

Thus, from the system of equations (5), having dimension $2N \times 2N$, where N — the number of terms retained during calculations in the field expansions (2), we obtained 2 systems with dimension $N \times N$. Next, for a single particle, it is easy to collect the expansion coefficients of the scattered field from two solutions, which have the form $\mathbf{Z}_1^{sca} = \{\mathbf{Z}_{1,U}^{sca}, \mathbf{Z}_{1,V}^{sca}\}$ and $\mathbf{Z}_2^{sca} = \{\mathbf{Z}_{2,U}^{sca}, \mathbf{Z}_{2,V}^{sca}\}$ and determine any optical characteristics of the particle. For ensembles of particles, both obtained T matrices, which do not contain zero elements, should be transformed, as described in the work [8], until two reduced analogues of the standard T-matrix are found, and only at this stage they should be combined into one, final.

Let us add that when using trigonometric functions of the azimuthal angle φ in the basis functions (4), the potential V^{in} of the incident plane wave is equal to zero [6] and, therefore, the vector of expansion coefficients $\mathbf{Z}_V^{in} = 0$. A modification of the system of equations (5), using this fact, allows to make numerical calculations even more economical.

Let us write the first equation of the system (5) taking into account the block diagram (6), (7)

$$-\begin{pmatrix} \alpha_{U,31} & \alpha_{V,31} \\ \beta_{U,31} & \beta_{V,31} \end{pmatrix} \begin{pmatrix} \mathbf{Z}_U^{int} \\ \mathbf{Z}_V^{int} \end{pmatrix} = \begin{pmatrix} \mathbf{Z}_U^{in} \\ 0 \end{pmatrix}. \tag{31}$$

Let us represent the second equation of this system in the form

$$\mathbf{Z}_V^{int} = -\left(\beta_{V,31}\right)^{-1} \beta_{U,31}\mathbf{Z}_U^{int}. \tag{32}$$

Now the first equation of system (31) can be solved with respect to the vector $\mathbf{Z}_U^{int}$

$$\mathbf{Z}_U^{int} = \left[\alpha_{V,31}\left(\beta_{V,31}\right)^{-1}\beta_{U,31} - \alpha_{U,31}\right]^{-1} \mathbf{Z}_U^{in} = A_U^{-1}\mathbf{Z}_U^{in}, \tag{33}$$

and after simple transformations we obtain a solution for the vector $\mathbf{Z}_V^{int}$

$$\mathbf{Z}_V^{int} = \left[\alpha_{U,31}\left(\beta_{U,31}\right)^{-1}\beta_{V,31} - \alpha_{V,31}\right]^{-1} \mathbf{Z}_U^{in} = A_V^{-1}\,\mathbf{Z}_U^{in}, \tag{34}$$

where notations are introduced for matrices written in square brackets.

The final solution for the expansion coefficients of the scattered field will be found from the second equation of the system (5) taking into account relations (33), (34):

$$\mathbf{Z}_U^{sca} = \left(\alpha_{U,11}A_U^{-1} + \alpha_{V,11}A_V^{-1}\right) \mathbf{Z}_U^{in},$$
$$\mathbf{Z}_V^{sca} = \left(\beta_{U,11}A_U^{-1} + \beta_{V,11}A_V^{-1}\right) \mathbf{Z}_U^{in}. \tag{35}$$

A simplification of the original solution is that instead of inverting the block matrix $\tilde{A}_{31}$, you need to find four inverse

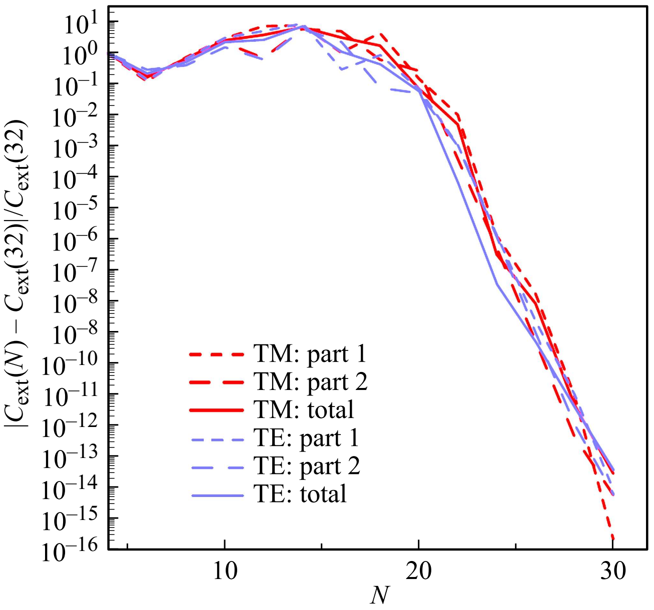

Figure 1. Convergence of extinction cross sections C_{ext} with increasing number of terms taken into account in field expansions, N, for TE and TM modes in the case of the initial system $2N \times 2N$ and each of the two systems $N \times N$ obtained after eliminating zeros. An oblate spheroid with $a/b = 2$, $\tilde{m} = 1.5$ and $x_{\text{V}} = 30$ with $\alpha = 45^\circ$ is reviewed.

matrices A_{U}^{-1}, A_{V}^{-1}, β_{U}^{-1}, β_{V}^{-1}, the dimension of which is half the original one.

Certainly, as part of this diagram, the exclusion of zero elements in the matrices of the system (35) can also be done. Dividing the coefficient vectors into two parts, as was done above, we obtain $(j = 1, 2)$

$$\mathbf{Z}^{\text{sca}}_{j,\text{U}} = \left(\alpha_{j,\text{U},11} A^{-1}_{j,\text{U}} + \alpha_{3-j,\text{V},11} A^{-1}_{3-j,\text{V}}\right) \mathbf{Z}^{\text{in}}_{j,\text{U}},$$

$$\mathbf{Z}^{\text{sca}}_{3-j,\text{V}} = \left(\beta_{3-j,\text{U},11} A_{j,\mathbf{U}_{11}} A^{-1}_{j,\text{U}} + \beta_{j,\text{V},11} A^{-1}_{3-j,\mathbf{V}}\right) \mathbf{Z}^{\text{in}}_{j,\text{U}}, \tag{36}$$

where

$$A_{j,\text{U}} = \alpha_{3-j,\text{V},31} \left(\beta_{j,\text{V},31}\right)^{-1} \beta_{3-j,\text{U},31} - \alpha_{j,\text{U},31},$$

$$A_{3-j,\text{V}} = \alpha_{j,\text{U},31} \left(\beta_{3-j,\text{U},31}\right)^{-1} \beta_{j,\text{V},31} - \alpha_{3-j,\text{V},31}. \tag{37}$$

The expressions for matrices $\alpha_{j,\text{X},ik}$ and $\beta_{j,\text{X},ik}$ are the same as above (27)–(30).

Let us note that a simple modification of the system of equations, described by the relations (31)–(37), additionally accelerates the calculations in a noticeable way.

4. Results of numerical tests

We applied the zero-elimination approach proposed in Section 3 to the algorithm outlined in [8] and briefly described in Section 2. Using the algorithm in its original form and after modification, excluding zero elements in the matrices of system (5) and dividing the latter into two systems of half the size, calculations of the optical properties of spheroids of various shapes with different refractive index $\tilde{m}$ were carried out. The diffraction parameter of the particles varied $x_{\text{V}} = 2\pi r_{\text{V}}/\lambda$, where r_{V} — the radius of the sphere, the volume of which is equal to the volume of the spheroid, λ — the wavelength of the radiation, and the minimum number of terms in the fields expansion N_{min} was determined, allowing one to obtain cross sections with an error of approximately 10^{-6}. The accuracy of the calculated sections was assessed as in [8].

The dependence of the computation time on N_{min} is most important for discussing the effectiveness of the proposed modification of the algorithm from [8]. However, before this, the question of the convergence of solutions in the original and modified algorithms for each of the modes with an increase in the number of terms taken into account in the field expansions N should be reviewed. Standard results of such review are presented in Fig. 1. They illustrate the convergence of extinction cross sections C_{ext} for an oblate spheroid with semi-axial ratio $a/b = 2$, refraction index $\tilde{m} = 1.5$, diffraction parameter $x_{\text{V}} = 30$ ($N_{\text{min}} = 32$) at oblique incidence of radiation (the angle between the symmetry axis of the particle and the wave vector $\alpha = 45^\circ$). These results, as well as our study as a whole, show that for each mode the rate of convergence of solutions of both reduced systems is almost similar to the rate of convergence for the original system.

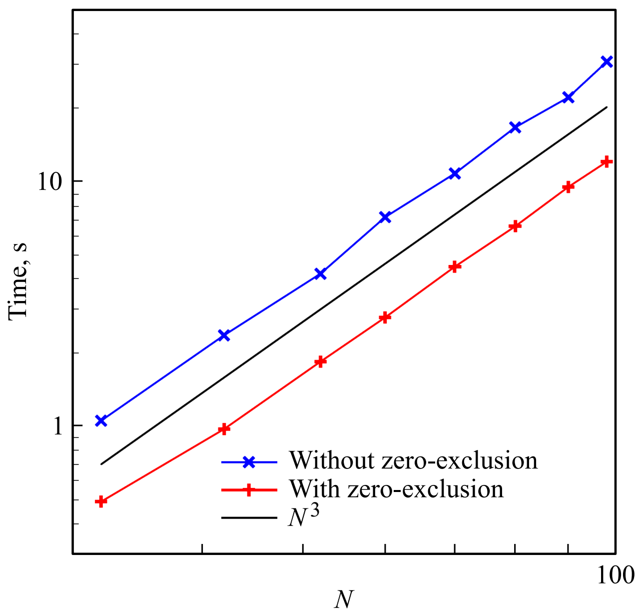

Figure 2. Time to solve the problem of light scattering (for one azimuthal mode) by oblate spheroids with $a/b = 2$, $\tilde{m} = 1.5$, $\alpha = 45^\circ$ and different diffraction parameters x_{V}, which required taking into account the $N = N_{\text{min}} \approx x_{\text{V}}$ E terms of the field expansion to achieve a section error of the order of 10^{-6}. Crosses and pluses — calculations without and with the exclusion of zeros, respectively.

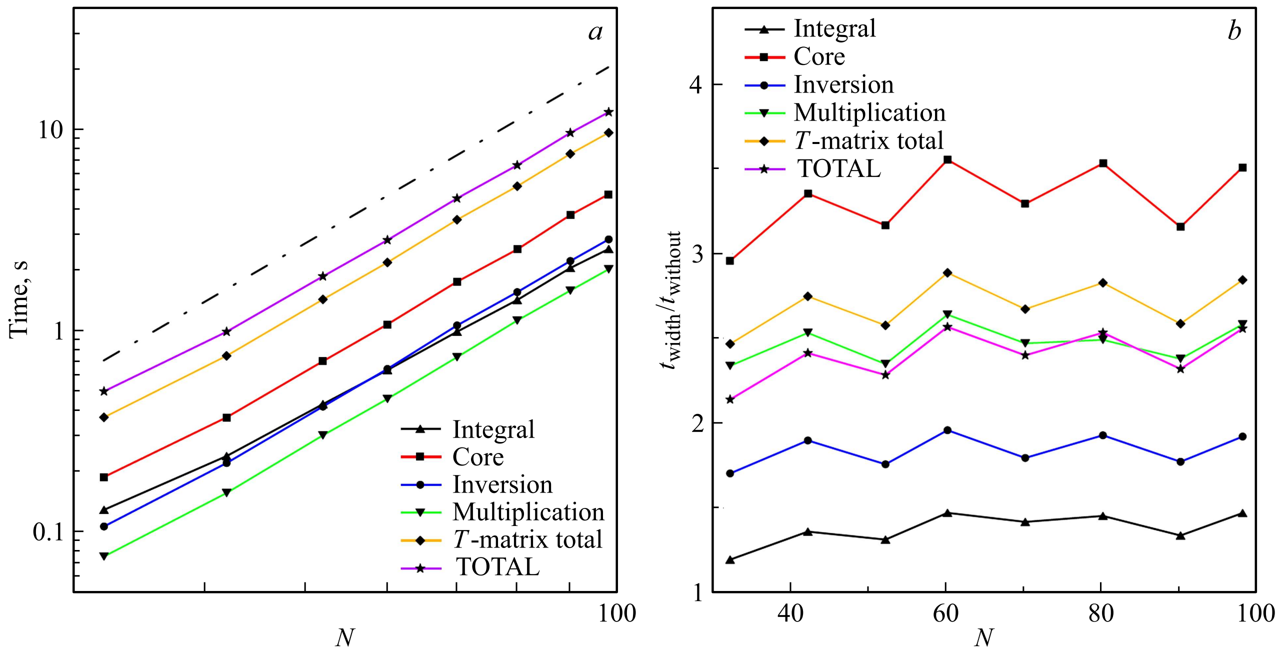

Figure 3. Left: time required for calculations after eliminating zero elements in different parts of the algorithm (see text for more details) for the same spheroids as in Fig. 2 with different numbers of terms taken into account in the field expansion, $N = N_{\min}$. The dot-dash line shows the N^3 relationship. Right: ratio of calculation times without exclusion (t_{with}) and with exclusion (t_{without}) of zero elements in different parts of the algorithm for the same spheroids with different numbers of terms $N = N_{\min}$.

After analyzing these and other results obtained, we found the following. The time for solving the problem (calculating part of the standard T matrix) for one azimuthal mode (one number m) depends on the number of terms of the expansion (system size) $N_{\min}$ approximately as $N^3_{\min}$ with $N_{\min} > 40$. In this case, the acceleration due to the application of the proposed approach, i.e. the ratio of calculation times without exclusion and with exclusion of zero elements is on average 2.5.

These conclusions are illustrated in Fig. 2, in which we showed the time for calculating cross-sections and T-matrices for oblate spheroids with $a/b = 2$, $\tilde{m} = 1.5$, $\alpha = 45°$ and different x_V when using a PC with an Intel Core i7 2.7 GHz processor (1 core was used). Particles of different sizes were reviewed in the range $x_V = 30 - 100$ (for given parameter values $N_{\min} \approx x_V$).

Let us note that to completely solve the problem it is required to review $m_{\max}$ azimuthal modes (2)–(4), where $m_{\max}$ is largely determined similarly to $N_{\min}$ by reviewing the internal convergence of the calculation results. For spheroids of the same shape with the same refraction index, it is known to be $m_{\max}/N_{\min} \approx \text{const}$, and therefore the total computation time for one particle is $t \sim N^4_{\min}$. However, the convergence of the results with increasing azimuthal number m (and, consequently, the value of $m_{\max}$) is obviously not affected by the considered division of the systems into 2 parts.[1] Therefore, the maximum acceleration with this approach should not be $2^4/2 = 8$, but approximately $2^p/2 \approx 3.3 - 4$, where, depending on the optimization of matrix multiplication and inversion, $p \approx 2.7 - 3$.

Further, it is obvious that the approach with excluding zeros should have different effects on different blocks of the algorithm, and accordingly, the actual acceleration of calculations within the approach should be significantly less than the maximum noted above. We have divided the algorithm into the following parts: 1) integrals — calculating matrix elements $\Delta_{i,j}, \Gamma_{i,j}, K_{i,j}, E_{i,j}$ ($i = 1, 2$; $j = 1, 2$), using the series representation of these integrals [12]; 2) core — calculation of matrix elements $\tilde{A}_{ik}$ ($i = 1, 3; k = 1$) using the following formulae (7), (8)–(11) and etc.; 3) inversion — matrix inversion $\tilde{A}_{31}$; 4) multiplication — matrix multiplication $\tilde{A}_{11}\tilde{A}_{31}^{-1}$.

The operating times of these blocks for spheroidal particles, which were reviewed in Fig. 2, are shown in the left panel of Fig. 3. As can be seen, with $N_{\min} > 40$ the operating times of all blocks are proportional to $N^3_{\min}$ (despite the fact that optimization was used in the Fortran compiler). The relative contribution of blocks to the total calculation time (in the figure — TOTAL) weakly depends on $N_{\min}$ and is: integrals — $\sim 20\%$, multiplication — $\sim 15\%$, inversion — $\sim 25\%$, core — $\sim 40\%$. The last three are designated in the figure as T-matrix total and add up to $\sim 80\%$.

Certainly, the application of the proposed approach gives different effects for different blocks (see the right panel of Fig. 3): the acceleration is minimal for integrals (~ 1.3) and maximum for core (~ 3.4). In the first case, the

[1] Accordingly, Figs. 2, 3 shows the times for the $m = m_{\max}$ mode.

formulae involve matrix inversion, which, however, takes only a small part of the time. In the second case we have almost maximum acceleration (see discussion above). Matrix inversion was slightly accelerated ($\sim$1.8), since in the program it was initially done in blocks using the Frobenius formula. Nevertheless, on average, the acceleration coefficient is consistently on the order of 2.5 both for the particles reviewed and for spheroids of a different shape and with a different refraction index.

Let us note that the proposed approach accelerates calculations in all blocks, and not just in the most expensive core block. On the other hand, the obtained assessment of the acceleration coefficient shows that the simple acceleration of calculations described at the end of Section 3 can be as important as eliminating zeros.

It is appropriate to compare the obtained effect with the acceleration of calculations in this problem when using standard MPI parallelization of calculations. In [8] it was found that the parallelized code ran ~ 4 times faster with 8 processors than the original. A simple assessment using Amdahl's law then shows that the maximum acceleration is by eliminating zeros, supplemented by the simplification described at the end of Section 3.

5. Conclusion

When analytically solving the problem of light scattering by a particle with a plane of symmetry using methods based on the fields expansion in the corresponding basis functions, systems of linear equations arise for unknown scattered field coefficients. In these systems, half of the matrix elements are zero. We proposed to use this fact for the acceleration of the calculations. By excluding the zero elements, we obtained two linear systems half the size of the original one.

This general approach is applied to a recent solution to the problem of light scattering by spheroids obtained by EBCM with a non-standard spheroidal basis. Numerical calculations have shown that the approach accelerates the calculations by approximately 2.5 times, which is comparable to the acceleration provided by parallelization of calculations, especially if we further simplify the systems that arise for the TE and TM modes.

Let us note that the proposed approach can be applied to non-axisymmetric scatterers, as well as layered particles by choosing a suitable spherical, cylindrical or spheroidal basis.

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Conflict of interest

The authors declare that they have no conflict of interest.

References

[1] C.F. Bohren, D.R. Huffman. *Absorption and scattering of light by small particles* (John Wiley, New York, 1983). DOI: 10.1002/9783527618156

[2] F.M. Kahnert, J.J. Stamnes, K. Stamnes. J. Quant. Spectrosc. Rad. Transf., **74**, 167–182 (2002). DOI: 10.1016/S0022-4073(01)00194-7

[3] P. Piedra, A. Kalume, E. Zubko et al. J. Quant. Spectrosc. Rad. Transf., **231**, 140–156 (2019). DOI: 10.1016/j.jqsrt.2019.04.013

[4] M.I. Mishchenko, J.W. Hovenier, L.D. Travis. *Light scattering by nonspherical particles: theory, measurements, and applications* (Academic Press, San Diego, 2000).

[5] B. Sun, G.W. Kattawar, P. Yang, X. Zhang. Appl. Sci., **8**, 2686 (2018). DOI: 10.3390/app8122686

[6] V.G. Farafonov, V.B. Il'in. Light Scatt. Rev., **1**, 125–177 (2006). DOI: 10.1007/3-540-37672-0_4

[7] P.W. Barber, S.C. Hill. *Light scattering by particles: computational methods* (World Scientific, Singapore, 1990). DOI: 10.1142/0784

[8] V.B. Il'in, D.G. Turichina, V.G. Farafonov et al. J. Quant. Spectrosc. Rad. Transf., **311**, 108759 (2023). DOI: 10.1016/j.jqsrt.2023.108759

[9] C. Flammer. *Spheroidal wave functions* (Stanford Univ. Press, Stanford, 1957).

[10] J. Meixner, F.W. Schäfke. *Mathieusche Funktionen and Sphäroidfunktionen* (Springer, Berlin, 1954).

[11] I.V. Komarov, L.I. Ponomarev, S.Yu. Slavyanov. *Sferoidalnyye i kulonovskiye sferoidalnyye funktsii* (Nauka, M., 1976) (in Russian).

[12] N.V. Voshchinnikov, V.G. Farafonov. Astrophys. Spa. Sci., **204**, 19–86 (1993). DOI: 10.1007/BF00658095

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